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Theoretical study of the self-assembly of Janus Bottlebrush Polymers from A-Branch-B Diblock Macromonomers KARIM GADELRAB, ALFREDO ALEXANDER-KATZ, Department of Materials Science and Engineering, MIT, LABORATORY FOR THEORETICAL SOFT MATERIALS TEAM — The self-assembly of block copolymers BCP has provided an impressive control over the nanoscale structure of soft matter. While the main focus of the research in the field has been directed towards simple linear diblocks, the development of advanced polymer architecture provided improved performance and access to new structures. In particular, bottlebrush BCPs (BBCPs) have interesting characteristics due to their dense functionality, high molecular weight, low levels of entanglement, and tendency to efficiently undergo rapid bulk phase separation. In this work, we are interested in theoretically studying the self-assembly of Janus-type "A-*branch*-B" BBCPs where A and B blocks can phase separate with the bottlebrush polymer backbone serving as the interface between the two blocks. Hence, the polymer backbone adds an extra constraint on the equilibrium spacing between neighboring linear diblock chains. In this regard, the segment length of the backbone separating the AB junctions has a direct effect of the observed domain spacing and effective segregation strength of the AB blocks. We employ self-consistent field theoretic SCFT simulations to capture the effect of volume fraction of different constituents and construct a phase diagram of the accessible morphologies of these BBCPs.

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